

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:sssptal610jxm

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

STN
modified

10-25-02

* * * * * Welcome to STN International * * * * *

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America
NEWS 2 Apr 08 "Ask CAS" for self-help around the clock
NEWS 3 Apr 09 BEILSTEIN: Reload and Implementation of a New Subject Area
NEWS 4 Apr 09 ZDB will be removed from STN
NEWS 5 Apr 19 US Patent Applications available in IFICDB, IFIPAT, and
IFIUDB
NEWS 6 Apr 22 Records from IP.com available in CAPLUS, HCAPLUS, and
ZCAPLUS
NEWS 7 Apr 22 BIOSIS Gene Names now available in TOXCENTER
NEWS 8 Apr 22 Federal Research in Progress (FEDRIP) now available
NEWS 9 Jun 03 New e-mail delivery for search results now available
NEWS 10 Jun 10 MEDLINE Reload
NEWS 11 Jun 10 PCTFULL has been reloaded
NEWS 12 Jul 02 FOREGE no longer contains STANDARDS file segment
NEWS 13 Jul 22 USAN to be reloaded July 28, 2002;
saved answer sets no longer valid
NEWS 14 Jul 29 Enhanced polymer searching in REGISTRY
NEWS 15 Jul 30 NETFIRST to be removed from STN
NEWS 16 Aug 08 CANCERLIT reload
NEWS 17 Aug 08 PHARMAMarketLetter(PHARMAML) - new on STN
NEWS 18 Aug 08 NTIS has been reloaded and enhanced
NEWS 19 Aug 19 Aquatic Toxicity Information Retrieval (AQUIRE)
now available on STN
NEWS 20 Aug 19 IFIPAT, IFICDB, and IFIUDB have been reloaded
NEWS 21 Aug 19 The MEDLINE file segment of TOXCENTER has been reloaded
NEWS 22 Aug 26 Sequence searching in REGISTRY enhanced
NEWS 23 Sep 03 JAPIO has been reloaded and enhanced
NEWS 24 Sep 16 Experimental properties added to the REGISTRY file
NEWS 25 Sep 16 Indexing added to some pre-1967 records in CA/CAPLUS
NEWS 26 Sep 16 CA Section Thesaurus available in CAPLUS and CA
NEWS 27 Oct 01 CASREACT Enriched with Reactions from 1907 to 1985
NEWS 28 Oct 21 EVENTLINE has been reloaded
NEWS 29 Oct 24 BEILSTEIN adds new search fields
NEWS 30 Oct 24 Nutraceuticals International (NUTRACEUT) now available on
STN

NEWS EXPRESS October 14 CURRENT WINDOWS VERSION IS V6.01,
CURRENT MACINTOSH VERSION IS V6.0a(ENG) AND V6.0Ja(JP),
AND CURRENT DISCOVER FILE IS DATED 01 OCTOBER 2002
NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS INTER General Internet Information
NEWS LOGIN Welcome Banner and News Items
NEWS PHONE Direct Dial and Telecommunication Network Access to STN
NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 15:24:12 ON 25 OCT 2002

=> fil reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 15:24:29 ON 25 OCT 2002

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STRUCTURE FILE UPDATES: 23 OCT 2002 HIGHEST RN 464874-85-9

DICTIONARY FILE UPDATES: 23 OCT 2002 HIGHEST RN 464874-85-9

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:

<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=>

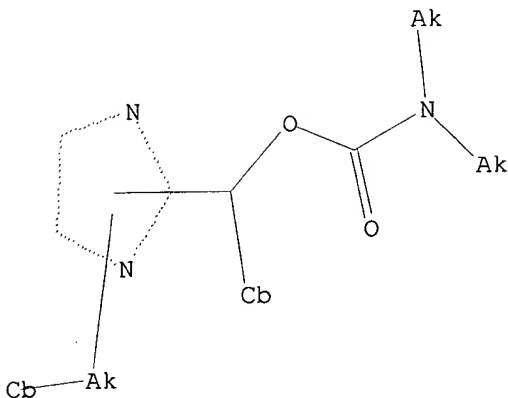
Uploading 09862808 electb.str

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

```
=> s ll ful
FULL SEARCH INITIATED 15:25:35 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 55519 TO ITERATE
```

```
100.0% PROCESSED    55519 ITERATIONS
SEARCH TIME: 00.00.04
```

5 ANSWERS

L2 5 SEA SSS FUL L1

```
=> s l2 and caplus/lc
      24954858 CAPLUS/LC
L3      5 L2 AND CAPLUS/LC
```

=> fil caplus

COST IN U.S. DOLLARS

SINCE FILE

ENTRY

TOTAL

SESSION

FULL ESTIMATED COST

144.66

144.87

FILE 'CAPLUS' ENTERED AT 15:25:52 ON 25 OCT 2002
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FILE COVERS 1907 - 25 Oct 2002 VOL 137 ISS 18
FILE LAST UPDATED: 24 Oct 2002 (20021024/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

=> s l2 ful

L4 2 L2

=> d l4 1-2 ibib abs

L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2001:904116 CAPLUS
DOCUMENT NUMBER: 136:37606
TITLE: Synthesis of 2-substituted azoles via multicomponent reactions.

INVENTOR(S): Hlaasta, Dennis
PATENT ASSIGNEE(S): Ortho-McNeil Pharmaceutical, Inc., USA
SOURCE: PCT Int. Appl., 80 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

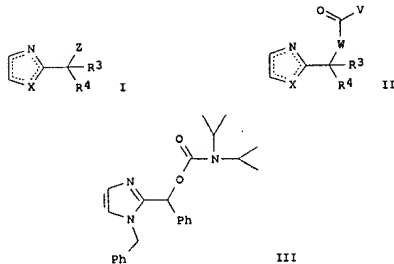
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001094318	A2	20011213	WO 2001-US16727	20010522
WO 2001094318	A3	20020718		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

US 2002042520 A1 20020411 US 2001-362208 20010522
PRIORITY APPLN. INFO.: US 2000-209252P P 200000605
OTHER SOURCE(S): CASREACT 136:7606; MARPAT 136:37606
GI

provisional

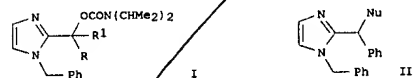
L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2002 ACS (Continued)



AB Title compds. (I; X = NH, NRa, S; Z = ORa, NRaRb, SR, cyano, N3, etc.; R3 = H, alkyl, (substituted) aralkyl, cycloalkyl, fluoroalkyl, COR, CO2R, etc.; R4 = alkyl, aryl, aralkyl, cycloalkyl, fluoroalkyl, alkenyl, alkynyl, COR, etc.; Ra, Rb = H, R, CO2R, COR, SO2R, SOR, etc.; R = alkyl, (substituted) aralkyl, cycloalkyl, adamantyl, norbornyl, fluoroalkyl, heterocyclyl], were prepd. by treatment of the corresponding unsubstituted azoles with ACOV (A = F, Cl, Br, OCOCH3; V = sterically hindered group) and then with R3C(:W)R4 (W = O, NSO2R, NSOR, NCO2R, NR; R as above) to give compds. (II; variables as above) followed by optional treatment of II with ZH (Z as above). Thus, 1-benzylimidazole in MeCN at 0.degree. was treated sequentially with diisopropylcarbamoyl chloride in MeCN, PhCHO, and diisopropylethylamine followed by 24 h reflux to give 78% title compd. (III).

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2000:910341 CAPLUS
DOCUMENT NUMBER: 134:193376
TITLE: Novel use of imidazolium ylides in an efficient synthesis of 2-substituted imidazoles
AUTHOR(S): Hlaasta, Dennis J.
CORPORATE SOURCE: Drug Discovery The R.W. Johnson Pharmaceutical Research Institute, Spring House, PA, 15477-0776, USA
SOURCE: Organic Letters (2001) 3(2), 157-159
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:193376
GI



AB A new reaction of imidazoles was discovered involving the formation of an imidazolium ylide, which on trapping with various electrophiles afforded diverse 2-substituted imidazoles I (R = CMe3, R1 = H; R = Ph, R1 = H; R = Ph, R1 = CF3; etc.). The facile, convenient reaction conditions when compared to the existing procedures make this reaction the method of choice in the prepn. of 2-substituted imidazoles. Moreover, the reaction differs from the reported methods since the products contain an .alpha.-substituent that is transformed by solvolysis chem. into further functionalized derivs. II (Nu = H, MeO, Eto, etc.).
REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

Apps get priority
date of 6.5.00
plus 1 yr behind = 6.5.01
∴ Date not good

=> fil reg
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
5.77	150.64

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-1.24	-1.24

CA SUBSCRIBER PRICE

FILE 'REGISTRY' ENTERED AT 15:27:53 ON 25 OCT 2002
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STRUCTURE FILE UPDATES: 23 OCT 2002 HIGHEST RN 464874-85-9
DICTIONARY FILE UPDATES: 23 OCT 2002 HIGHEST RN 464874-85-9

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

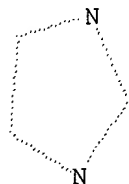
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP
PROPERTIES for more information. See STNote 27, Searching Properties
in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=>
Uploading react 1.str

L5 STRUCTURE UPLOADED

=> d
L5 HAS NO ANSWERS
L5 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 15 ful
FULL SEARCH INITIATED 15:28:09 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - >1,000,000 TO ITERATE

< 40.0% PROCESSED 400000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.09

343630 ANSWERS

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: EXCEEDS 1000000
PROJECTED ANSWERS: EXCEEDS 1000000

L6 343630 SEA SSS FUL L5

=>

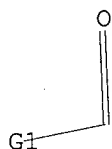
Uploading react2.str

L7 STRUCTURE UPLOADED

=> d

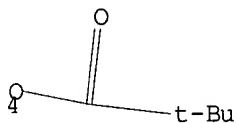
L7 HAS NO ANSWERS

L7 STR



F¹

Br 3 Cl 2



G1 [@1],[@2],[@3],[@4]

Structure attributes must be viewed using STN Express query preparation.

=> s 17 ful

FULL SEARCH INITIATED 15:31:36 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 203710 TO ITERATE

100.0% PROCESSED 203710 ITERATIONS
SEARCH TIME: 00.00.04

76465 ANSWERS

L8 76465 SEA SSS FUL L7

=> fil caplus

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
282.46	433.10

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-1.24

CA SUBSCRIBER PRICE

FILE 'CAPLUS' ENTERED AT 15:31:51 ON 25 OCT 2002
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FILE COVERS 1907 - 25 Oct 2002 VOL 137 ISS 18
FILE LAST UPDATED: 24 Oct 2002 (20021024/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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=> s 18

L9 148229 L8

=> s 16 ful

TOO MANY TERMS FOR FILE CROSSOVER IN L6

There are limits on the size of an answer set being crossed over from one file to another. Enter HELP CROSSOVER at an arrow prompt (=>) for specific information.

=> s 19 and 16 ful

TOO MANY TERMS FOR FILE CROSSOVER IN L6

There are limits on the size of an answer set being crossed over from

one file to another. Enter HELP CROSSOVER at an arrow prompt (=>) for specific information.

=> fil reg

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
0.79	433.89

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-1.24

CA SUBSCRIBER PRICE

FILE 'REGISTRY' ENTERED AT 15:33:18 ON 25 OCT 2002
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STRUCTURE FILE UPDATES: 23 OCT 2002 HIGHEST RN 464874-85-9
DICTIONARY FILE UPDATES: 23 OCT 2002 HIGHEST RN 464874-85-9

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

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<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=>

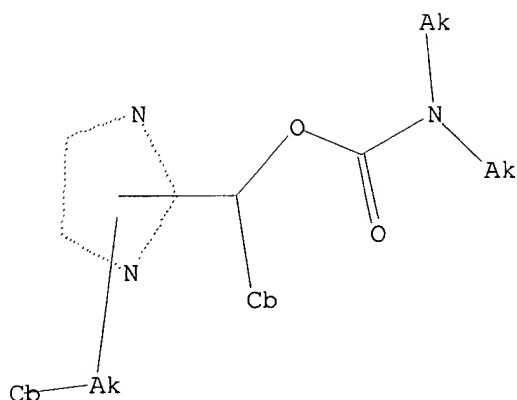
Uploading 09862808 electb.str

L10 STRUCTURE UPLOADED

=> d

L10 HAS NO ANSWERS

L10 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l10 ful
 FULL SEARCH INITIATED 15:34:06 FILE 'REGISTRY'
 FULL SCREEN SEARCH COMPLETED - 55519 TO ITERATE

100.0% PROCESSED 55519 ITERATIONS 5 ANSWERS
 SEARCH TIME: 00.00.04

L11 5 SEA SSS FUL L10

=> fil caplus		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	140.66	574.55
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-1.24

FILE 'CAPLUS' ENTERED AT 15:34:13 ON 25 OCT 2002
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FILE COVERS 1907 - 25 Oct 2002 VOL 137 ISS 18
FILE LAST UPDATED: 24 Oct 2002 (20021024/ED)

This file contains CAS Registry Numbers for easy and accurate
substance identification.

CAS roles have been modified effective December 16, 2001. Please
check your SDI profiles to see if they need to be revised. For
information on CAS roles, enter HELP ROLES at an arrow prompt or use
the CAS Roles thesaurus (/RL field) in this file.

=> s l11 ful
L12 2 L11

=> s l12 and l9
L13 2 L12 AND L9

=> d l13 1-2 ibib abs hitstr

L13 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2002 ACS

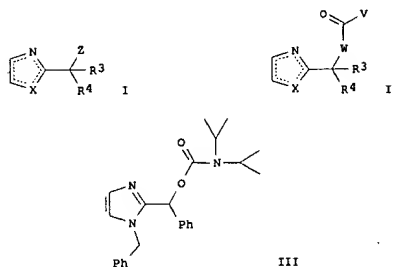
ACCESSION NUMBER: 2001:904116 CAPLUS
DOCUMENT NUMBER: 136:37606
TITLE: Synthesis of 2-substituted azoles via multicomponent reactions.
INVENTOR(S): Hiasta, Dennis
PATENT ASSIGNEE(S): Ortho-McNeil Pharmaceutical, Inc., USA
SOURCE: PCT Int. Appl., 80 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001094318	A2	20011213	WO 2001-US16727	20010522
WO 2001094318	A3	20020718		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
US 2002042520 A1 20020411 US 2001-862808 20010522
PRIORITY APPLN. INFO.: US 2000-209252P 20000605
OTHER SOURCE(S): CASREACT 136:37606; MARPAT 136:37606
GI

provisional.

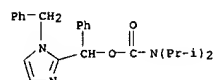
L13 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2002 ACS (Continued)



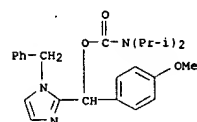
AB Title compds. [I: X = NH, NHa, S; Z = ORa, NRaRb, SR, cyano, N3, etc.; R3 = H, alkyl, (substituted) aralkyl, cycloalkyl, fluoroalkyl, COR, CO2R, etc.; R4 = alkyl, aryl, aralkyl, cycloalkyl, fluoroalkyl, alkenyl, alkynyl, COR, etc.; Ra, Rb = H, R, CO2R, COR, SO2R, SOR, etc.; R = alkyl, (substituted) aralkyl, cycloalkyl, adamantyl, norbornyl, fluoroalkyl, heterocyclyl], were prep'd. by treatment of the corresponding unsubstituted azoles with ACOV (A = F, Cl, Br, OCOCH3; V = sterically-hindered group) and then with R3C(W)R4 (W = O, NSO2R, NSOR, NCO2R, NR; R as above) to give compds. (II; variables as above) followed by optional treatment of II with ZH (Z as above). Thus, 1-benzylimidazole in MeCN at 0.degree. was treated sequentially with diisopropylcarbamoyl chloride in MeCN, PhCHO, and diisopropylethylamine followed by 24 h reflux to give 78% title compd. (III).

IT 327626-37-9P 327626-38-0P 327626-39-1P
327626-40-4P 380303-14-0P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(synthesis of 2-substituted azoles via multicomponent reactions)
RN 327626-37-9 CAPLUS
CN Carbamic acid, bis(1-methylethyl)-, phenyl[1-(phenylmethyl)-1H-imidazol-2-yl]methyl ester (9CI) (CA INDEX NAME)

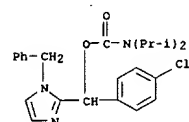
L13 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 327626-38-0 CAPLUS
CN Carbamic acid, bis(1-methylethyl)-, (4-methoxyphenyl)[1-(phenylmethyl)-1H-imidazol-2-yl]methyl ester (9CI) (CA INDEX NAME)

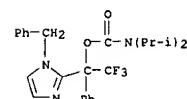


RN 327626-39-1 CAPLUS
CN Carbamic acid, bis(1-methylethyl)-, (4-chlorophenyl)[1-(phenylmethyl)-1H-imidazol-2-yl]methyl ester (9CI) (CA INDEX NAME)

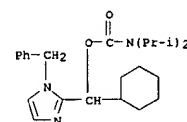


RN 327626-40-4 CAPLUS
CN Carbamic acid, bis(1-methylethyl)-, 2,2,2-trifluoro-1-phenyl-1-[1-(phenylmethyl)-1H-imidazol-2-yl]methyl ester (9CI) (CA INDEX NAME)

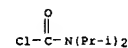
L13 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2002 ACS (Continued)



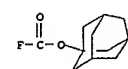
RN 380303-14-0 CAPLUS
CN Carbamic acid, bis(1-methylethyl)-, cyclohexyl[1-(phenylmethyl)-1H-imidazol-2-yl]methyl ester (9CI) (CA INDEX NAME)



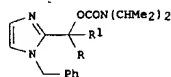
IT 19009-39-3, Diisopropylcarbamoyl chloride 62087-82-5
RL: RCT (Reactant); RACT (Reactant or Reagent)
(synthesis of 2-substituted azoles via multicomponent reactions)
RN 19009-39-3 CAPLUS
CN Carbamic chloride, bis(1-methylethyl)- (9CI) (CA INDEX NAME)



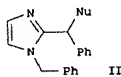
RN 62087-82-5 CAPLUS
CN Carbonyl fluoride, tricyclo[3.3.1.1.3,7]dec-1-yl ester (9CI) (CA INDEX NAME)



L13 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 2000:910341 CAPLUS
 DOCUMENT NUMBER: 134:193376
 TITLE: Novel use of imidazolium ylides in an efficient synthesis of 2-substituted imidazoles
 AUTHOR(S): Hlasta, Dennis J.
 CORPORATE SOURCE: Drug Discovery The R. W. Johnson Pharmaceutical Research Institute, Spring House, PA, 19477-0776, USA
 SOURCE: Organic Letters (2001), 7(2), 157-159
 CODEN: ORLEFF; ISSN: 1523-7060
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 134:193376
 GI



I



II

AB A new reaction of imidazoles was discovered involving the formation of an imidazolium ylide, which on trapping with various electrophiles afforded diverse 2-substituted imidazoles I (R = CMe3, R1 = H; R = Ph, R1 = H; R = Ph, R1 = CF3; etc.). The facile, convenient reaction conditions when compared to the existing procedures make this reaction the method of choice in the prepn. of 2-substituted imidazoles. Moreover, the reaction differs from the reported methods since the products contain an alpha.-substituent that is transformed by solvolysis chem. into further functionalized derivs. II (Nu = H, MeO, Eto, etc.).
 IT 98-88-4, Benzoyl chloride 3282-30-2, Pivaloyl chloride 19009-39-3, Diisopropylcarbonyl chloride
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (prepn. of imidazole derivs. by alkylation of imidazolium ylides)
 RN 98-88-4 CAPLUS
 CN Benzoyl chloride (8CI, 9CI) (CA INDEX NAME)



L13 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2002 ACS (Continued)

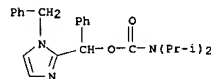
RN 3282-30-2 CAPLUS
 CN Propanoyl chloride, 2,2-dimethyl- (9CI) (CA INDEX NAME)



RN 19009-39-3 CAPLUS
 CN Carbamic chloride, bis(1-methylethyl)- (9CI) (CA INDEX NAME)

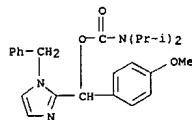


IT 327626-37-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. of imidazole derivs. by alkylation of imidazolium ylides)
 RN 327626-37-9 CAPLUS
 CN Carbamic acid, bis(1-methylethyl)-, phenyl[1-(phenylmethyl)-1H-imidazol-2-yl]methyl ester (9CI) (CA INDEX NAME)

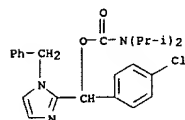


IT 327626-38-0P 327626-39-1P 327626-40-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of imidazole derivs. by alkylation of imidazolium ylides)
 RN 327626-38-0 CAPLUS
 CN Carbamic acid, bis(1-methylethyl)-, (4-methoxyphenyl)[1-(phenylmethyl)-1H-imidazol-2-yl]methyl ester (9CI) (CA INDEX NAME)

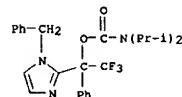
L13 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 327626-39-1 CAPLUS
 CN Carbamic acid, bis(1-methylethyl)-, (4-chlorophenyl)[1-(phenylmethyl)-1H-imidazol-2-yl]methyl ester (9CI) (CA INDEX NAME)



RN 327626-40-4 CAPLUS
 CN Carbamic acid, bis(1-methylethyl)-, 2,2,2-trifluoro-1-phenyl-1-[1-(phenylmethyl)-1H-imidazol-2-yl]ethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
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FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
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CA SUBSCRIBER PRICE

STN INTERNATIONAL LOGOFF AT 15:34:46 ON 25 OCT 2002

Connecting via Winsock to STN

STN
Inventor

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PASSWORD:

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10-25-02

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NEWS 1 Web Page URLs for STN Seminar Schedule - N. America
NEWS 2 Apr 08 "Ask CAS" for self-help around the clock
NEWS 3 Apr 09 BEILSTEIN: Reload and Implementation of a New Subject Area
NEWS 4 Apr 09 ZDB will be removed from STN
NEWS 5 Apr 19 US Patent Applications available in IFICDB, IFIPAT, and
IFIUDB
NEWS 6 Apr 22 Records from IP.com available in CAPLUS, HCAPLUS, and
ZCAPLUS
NEWS 7 Apr 22 BIOSIS Gene Names now available in TOXCENTER
NEWS 8 Apr 22 Federal Research in Progress (FEDRIP) now available
NEWS 9 Jun 03 New e-mail delivery for search results now available
NEWS 10 Jun 10 MEDLINE Reload
NEWS 11 Jun 10 PCTFULL has been reloaded
NEWS 12 Jul 02 FOREGE no longer contains STANDARDS file segment
NEWS 13 Jul 22 USAN to be reloaded July 28, 2002;
saved answer sets no longer valid
NEWS 14 Jul 29 Enhanced polymer searching in REGISTRY
NEWS 15 Jul 30 NETFIRST to be removed from STN
NEWS 16 Aug 08 CANCERLIT reload
NEWS 17 Aug 08 PHARMAMarketLetter(PHARMAML) - new on STN
NEWS 18 Aug 08 NTIS has been reloaded and enhanced
NEWS 19 Aug 19 Aquatic Toxicity Information Retrieval (AQUIRE)
now available on STN
NEWS 20 Aug 19 IFIPAT, IFICDB, and IFIUDB have been reloaded
NEWS 21 Aug 19 The MEDLINE file segment of TOXCENTER has been reloaded
NEWS 22 Aug 26 Sequence searching in REGISTRY enhanced
NEWS 23 Sep 03 JAPIO has been reloaded and enhanced
NEWS 24 Sep 16 Experimental properties added to the REGISTRY file
NEWS 25 Sep 16 Indexing added to some pre-1967 records in CA/CAPLUS
NEWS 26 Sep 16 CA Section Thesaurus available in CAPLUS and CA
NEWS 27 Oct 01 CASREACT Enriched with Reactions from 1907 to 1985
NEWS 28 Oct 21 EVENTLINE has been reloaded
NEWS 29 Oct 24 BEILSTEIN adds new search fields
NEWS 30 Oct 24 Nutraceuticals International (NUTRACEUT) now available on
STN

NEWS EXPRESS October 14 CURRENT WINDOWS VERSION IS V6.01,
CURRENT MACINTOSH VERSION IS V6.0a(ENG) AND V6.0Ja(JP),
AND CURRENT DISCOVER FILE IS DATED 01 OCTOBER 2002
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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 14:56:42 ON 25 OCT 2002

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FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 14:56:49 ON 25 OCT 2002
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STRUCTURE FILE UPDATES: 23 OCT 2002 HIGHEST RN 464874-85-9
DICTIONARY FILE UPDATES: 23 OCT 2002 HIGHEST RN 464874-85-9

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

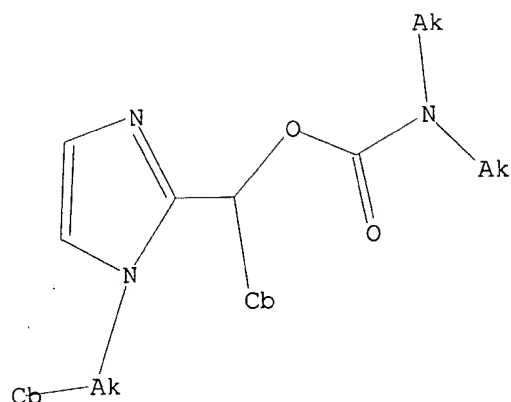
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=>
Uploading 09862808 elect.str

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

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FULL SCREEN SEARCH COMPLETED - 350 TO ITERATE
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100.0% PROCESSED 350 ITERATIONS
SEARCH TIME: 00.00.01
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5 ANSWERS

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L2 5 SEA SSS FUL L1
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FULL ESTIMATED COST          144.28          144.49
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FILE 'CAPLUS' ENTERED AT 14:57:23 ON 25 OCT 2002
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FILE COVERS 1907 - 25 Oct 2002 VOL 137 ISS 18
 FILE LAST UPDATED: 24 Oct 2002 (20021024/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

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L4          2 L2/P
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=> d 14 1-2 ibib abs hitstr
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L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2001:904116 CAPLUS

DOCUMENT NUMBER: 136:37606

TITLE: Synthesis of 2-substituted azoles via multicomponent

reactions.

INVENTOR(S): Hlasta, Dennis

PATENT ASSIGNEE(S): Ortho-McNeil Pharmaceutical, Inc., USA

SOURCE: PCT Int. Appl., 80 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001094318	A2	20011213	WO 2001-US16727	20010522
WO 2001094318	A3	20020718		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

US 2002042520 A1 20020411 US 2001-060063-20010522

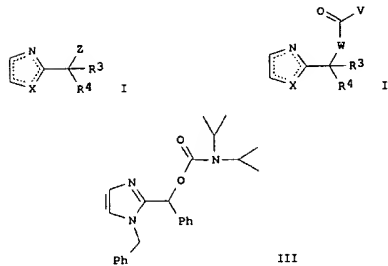
PRIORITY APPLN. INFO.: US 2000-209252P P 20000605

OTHER SOURCE(S): CASREACT 136:37606; MARPAT 136:37606

GI

provisional

L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2002 ACS (Continued)

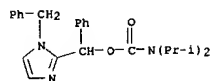


AB Title compds. (I; X = NH, NHa, S; Z = ORa, NRaRb, SR, cyano, N3, etc.; R3 = H, alkyl, (substituted) aralkyl, cycloalkyl, fluoroalkyl, COR, CO2R, etc.; R4 = alkyl, aryl, aralkyl, cycloalkyl, fluoroalkyl, alkenyl, alkynyl, COR, etc.; Ra, Rb = H, R, CO2R, COR, SO2R, SOR, etc.; R = alkyl, (substituted) aralkyl, cycloalkyl, adamantyl, norbornyl, fluoroalkyl, heterocyclyl, were prepd. by treatment of the corresponding unsubstituted azoles with ACOV (A = F, Cl, Br, COCMe3; V = sterically hindered group) and then with R3C(W)R4 (W = O, NSO2R, NSOR, NCOR, NCO2R, NR; R as above) to give compds. (II; variables as above) followed by optional treatment of II with ZH (Z as above). Thus, 1-benzylimidazole in MeCN at 0.degree. was treated sequentially with diisopropylcarbamoyl chloride in MeCN, PhCHO, and diisopropylethylamine followed by 24 h reflux to give 78% title compd. (III).

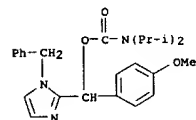
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327626-40-4P 380303-14-0P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(synthesis of 2-substituted azoles via multicomponent reactions)

RN 327626-37-9 CAPLUS
CN Carbamic acid, bis(1-methylethyl)-, phenyl[1-(phenylmethyl)-1H-imidazol-2-yl]methyl ester (9CI) (CA INDEX NAME)

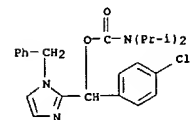
L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 327626-38-0 CAPLUS
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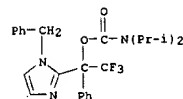


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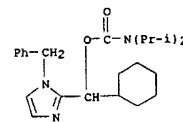


RN 327626-40-4 CAPLUS
CN Carbamic acid, bis(1-methylethyl)-, 2,2,2-trifluoro-1-phenyl-1-[(phenylmethyl)-1H-imidazol-2-yl]ethyl ester (9CI) (CA INDEX NAME)

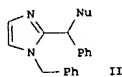
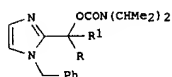
L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 380303-14-0 CAPLUS
CN Carbamic acid, bis(1-methylethyl)-, cyclohexyl[1-(phenylmethyl)-1H-imidazol-2-yl]methyl ester (9CI) (CA INDEX NAME)

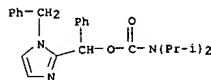


L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 2000:910341 CAPLUS
 DOCUMENT NUMBER: 134:193376
 TITLE: Novel use of imidazolium ylides in an efficient synthesis of 2-substituted imidazoles
 AUTHOR(S): Hlasta, Dennis J.
 CORPORATE SOURCE: Drug Discovery The R.W. Johnson Pharmaceutical Research Institute, Spring House, PA,
 19477-0776, USA
 SOURCE: Organic Letters (2001), 3(2), 157-159
 CODEN: ORLEF7; ISSN: 1523-7060
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 134:193376
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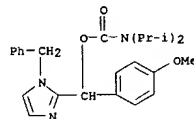


AB A new reaction of imidazoles was discovered involving the formation of an imidazolium ylide, which on trapping with various electrophiles afforded diverse 2-substituted imidazoles I (R = CMe₃, R₁ = H; R = Ph, R₁ = H; R = Ph, R₁ = CF₃; etc.). The facile, convenient reaction conditions when compared to the existing procedures make this reaction the method of choice in the prepn. of 2-substituted imidazoles. Moreover, the reaction differs from the reported methods since the products contain an .alpha.-substituent that is transformed by solvolysis chem. into further functionalized derivs. II (Nu = H, MeO, EtO, etc.).
 IT 327626-37-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. of imidazole derivs. by alkylation of imidazolium ylides)
 RN 327626-37-9 CAPLUS
 CN Carbamic acid, bis(1-methylethyl)-, phenyl[1-(phenylmethyl)-1H-imidazol-2-yl]methyl ester (9CI) (CA INDEX NAME)

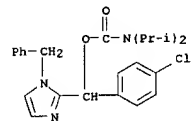
L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2002 ACS (Continued)



IT 327626-38-0P 327626-39-1P 327626-40-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of imidazole derivs. by alkylation of imidazolium ylides)
 RN 327626-38-0 CAPLUS
 CN Carbamic acid, bis(1-methylethyl)-, (4-methoxyphenyl)[1-(phenylmethyl)-1H-imidazol-2-yl]methyl ester (9CI) (CA INDEX NAME)

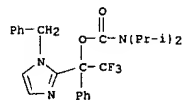


RN 327626-39-1 CAPLUS
 CN Carbamic acid, bis(1-methylethyl)-, (4-chlorophenyl)[1-(phenylmethyl)-1H-imidazol-2-yl]methyl ester (9CI) (CA INDEX NAME)



RN 327626-40-4 CAPLUS
 CN Carbamic acid, bis(1-methylethyl)-, 2,2,2-trifluoro-1-phenyl-1-[1-(phenylmethyl)-1H-imidazol-2-yl]ethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2002 ACS (Continued)



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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E3      16 --> DENG YIJUN/AU
E4      7       DENG YIKANG/AU
E5      1       DENG YILEI/AU
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L6      4 L5 AND AZOL?

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      (FILE 'HOME' ENTERED AT 14:56:42 ON 25 OCT 2002)

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      FILE 'REGISTRY' ENTERED AT 14:56:49 ON 25 OCT 2002

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L1      STRUCTURE UPLOADED
L2      5 S L1 FUL
L3      5 S L2 AND CAPLUS/LC

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      FILE 'CAPLUS' ENTERED AT 14:57:23 ON 25 OCT 2002

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L5      16 S (E3)
L6      4 S L5 AND AZOL?

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L7 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2002:808545 CAPLUS
TITLE: Synthetic Applications of Asolium Ylides to
a Traceless Solid-Phase Synthesis of
2-Substituted
Asoles
AUTHOR(S): Deng, Yijun; Hlasta, Dennis J.
CORPORATE SOURCE: Drug Discovery, Johnson Johnson Pharmaceutical
Research Development, Spring House, PA,
19477-0776,
USA
SOURCE: Organic Letters ACS ASAP
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A new approach for the prepn. of 2-substituted asole libraries
using a polystyrene-carbamyl chloride resin in a traceless fashion
is described. Asole substrates II are assembled in a one-pot
condensation reaction of asoles and aldehydes with a resin-bound
carbamyl chloride. Treatment of the asolyl-carbamate II with
boron trifluoride etherate under thermal or microwave-assisted
solvolysis
conditions afforded 2-substituted asoles.

L7 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:925485 CAPLUS
DOCUMENT NUMBER: 136:369622
TITLE: The synthesis of 2-substituted asoles
through a one-pot three-component reaction
Deng, Yijun; Hlasta, Dennis J.
Drug Discovery, The R. W. Johnson
Research Institute, Spring House, PA,
19477-0776, USA
SOURCE: Tetrahedron Letters (2002) 43(2), 189-192
CODEN: TETLAV; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB We have discovered a new reaction whereby 2-substituted asoles
are formed in the reaction of an asolium ylide with reactive
carbonyl compds. These products contain a leaving group in the
.alpha.-position, which on solvolysis in the presence of
nucleophiles
yield asoles with a variety of .alpha.-substituents. We have
developed new aspects of this chem. and expanded the scope to
include
imidazoles, thiazoles, benzimidazoles and triazoles, such that in
two
reaction steps a wide diversity of substitution patterns are
obtained.
REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE
FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE
RE FORMAT

Date is
no
good.

L7 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:640817 CAPLUS
TITLE: Novel traceless solid-phase synthesis of
2-substituted
asoles
AUTHOR(S): Deng, Yijun; Hlasta, Dennis J.
CORPORATE SOURCE: Drug Discovery, The R.W. Johnson Pharmaceutical
Research Institute, Spring House, PA, 19477,
USA
SOURCE: Abstracts of Papers, 222nd ACS National
Meeting,
Chicago, IL, United States, August 26-30, 2001,
(2001),
ORGN-454. American Chemical Society:
Washington, D.
C.
CODEN: 69BUZP
Conference: Meeting Abstract
LANGUAGE: English
AB Asoles, such as imidazole, are important heterocycle scaffolds
occurring in many drugs and biol. active compds. In the
accompanying
abstr., we describe a new reaction for the synthesis of
2-substituted
asoles via an asolium ylide. This reaction is ideal for
application to the traceless solid-phase synthesis of asole
libraries for high-throughput screening. In two reaction steps,
asoles are formed with three centers of diversity that are arrayed
in a compact structure around a single carbon atom. We have found
that in
one step 2-substituted asoles (I) are assembled on resin by
using a resin bound acid chloride. Solvolysis conditions result in
cleavage of the asole off the resin, presumably in the form of a
carbonium ion, which is then trapped with a variety of
nucleophiles. This
two step sequence affords a library of 2-substituted asoles (II)
with at least three centers of diversity.

L7 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:640398 CAPLUS
TITLE: New synthesis of 2-substituted asoles via a
three-component one-pot reaction
Deng, Yijun; Hlasta, Dennis J.
Drug Discovery, The R.W. Johnson Pharmaceutical
Research Institute, Spring House, PA, 19477,
USA
SOURCE: Abstracts of Papers, 222nd ACS National
Meeting,
Chicago, IL, United States, August 26-30, 2001,
(2001),
ORGN-035. American Chemical Society:
Washington, D.
C.
CODEN: 69BUZP
Conference: Meeting Abstract
LANGUAGE: English
AB A novel synthesis of 2-substituted asoles via an asolium
ylide has been discovered in our labs. In comparison with known
methods,
this new reaction is carried out under facile and convenient
conditions.
Moreover, we found that the product (I) is readily transformed by
direct
solvolysis/displacement chem. into a wide range of functionalized
asole derivs. (II). Our recent results in developing new aspects
and the scope of this reaction will be described.

No

No

```

=> E HLASTA DENNIS/AU 25
E1      1      HCLASS LISA J/AU
E2      7      HLASTA D J/AU
E3      7 --> HLASTA DENNIS/AU
E4      60     HLASTA DENNIS J/AU
E5      9      HLASTA DENNIS JOHN/AU
E6      7      HLASTALA M P/AU
E7      23     HLASTALA MICHAEL P/AU
E8      1      HLASTALA P/AU
E9      1      HLATER F/AU
E10     3      HLATKA A/AU
E11     1      HLATKEY GREGORY G/AU
E12     4      HLATKI MIKLOS/AU
E13     2      HLATKY ALEXANDER J/AU
E14     1      HLATKY G G/AU
E15     5      HLATKY GREGORY/AU
E16     34     HLATKY GREGORY G/AU
E17     17     HLATKY GREGORY GEORGE/AU
E18     2      HLATKY J/AU
E19     5      HLATKY JURAJ/AU
E20     4      HLATKY L/AU
E21     6      HLATKY L R/AU
E22     15     HLATKY LYNN/AU
E23     5      HLATKY LYNN R/AU
E24     1      HLATKY MARK/AU
E25     5      HLATKY MARK A/AU

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=> S (E2 OR E3 OR E4 OR E5)
      7 "HLASTA D J"/AU
      7 "HLASTA DENNIS"/AU
      60 "HLASTA DENNIS J"/AU
      9 "HLASTA DENNIS JOHN"/AU
L8      83 ("HLASTA D J"/AU OR "HLASTA DENNIS"/AU OR "HLASTA DENNIS J"/AU
OR "HLASTA DENNIS JOHN"/AU)

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=> s l8 and azol?
      7934 AZOL?
L9      6 L8 AND AZOL?

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=> d his

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(FILE 'HOME' ENTERED AT 14:56:42 ON 25 OCT 2002)

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FILE 'REGISTRY' ENTERED AT 14:56:49 ON 25 OCT 2002
L1      STRUCTURE UPLOADED
L2      5 S L1 FUL
L3      5 S L2 AND CAPLUS/LC

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FILE 'CAPLUS' ENTERED AT 14:57:23 ON 25 OCT 2002
L4      2 S L2/P
      E DENG YIJUN/AU 25
L5      16 S (E3)
L6      4 S L5 AND AZOL?
L7      4 S L6 NOT L4
      E HLASTA DENNIS/AU 25

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L8 83 S (E2 OR E3 OR E4 OR E5)
L9 6 S L8 AND AZOL?

=> s 19 not 14
L10 5 L9 NOT L4

=> s 110 not 19
L11 0 L10 NOT L9

=> d 110 1-5 ibib abs

L10 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 2002:808545 CAPLUS
 TITLE: Synthetic Applications of Asolium Ylides to a Traceless Solid-Phase Synthesis of 2-Substituted
 AUTHOR(S): Deng, Yijun; Mlaata, Dennis J.
 CORPORATE SOURCE: Drug Discovery, Johnson Johnson Pharmaceutical Research Development, Spring House, PA, 19477-0776, USA
 SOURCE: Organic Letters ACS ASAP
 CODEN: ORLEF7; ISSN: 1523-7060
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB A new approach for the prepn. of 2-substituted asole libraries using a polystyrene-carbamyl chloride resin in a traceless fashion is described. Asole substrates II are assembled in a one-pot condensation reaction of asoles and aldehydes with a resin-bound carbamyl chloride. Treatment of the asolyl-carbamate II with boron trifluoride etherate under thermal or microwave-assisted solvolysis conditions afforded 2-substituted asoles.

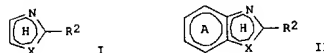
L10 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 2001:925485 CAPLUS
 DOCUMENT NUMBER: 136:369622
 TITLE: The synthesis of 2-substituted asoles through a one-pot three-component reaction
 AUTHOR(S): Deng, Yijun; Mlaata, Dennis J.
 CORPORATE SOURCE: Drug Discovery, The R. W. Johnson Research Institute, Spring House, PA, 19477-0776, USA
 SOURCE: Tetrahedron Letters (2002), 43(2), 189-192
 CODEN: TELEAY; ISSN: 0040-4039
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB We have discovered a new reaction whereby 2-substituted asoles are formed in the reaction of an asolium ylide with reactive carbonyl compds. These products contain a leaving group in the .alpha.-position, which on solvolysis in the presence of nucleophiles yield asoles with a variety of .alpha.-substituents. We have developed new aspects of this chem. and expanded the scope to include imidazoles, thiazoles, benzimidazoles and triazoles, such that in two reaction steps a wide diversity of substitution patterns are obtained.
 REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE
 RE FORMAT

L10 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 2001:904114 CAPLUS
 DOCUMENT NUMBER: 136:37605
 TITLE: Method for synthesis of substituted asole libraries
 INVENTOR(S): Mlaata, Dennis
 PATENT ASSIGNEE(S): Ortho-McNeill Pharmaceutical, Inc., USA
 SOURCE: PCT Int. Appl., 51 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001094317	A2	20011213	WO 2001-US16719	20010523
WO 2001094317	A3	20020411		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GE, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GN, GW, ML, MR, NE, NG, TD, TG
 US 2002077483 A1 20020620 US 2000-062749 20010522
 PRIORITY APPLN. INFO.: US 2000-209730 P 20000605
 OTHER SOURCE(S): CASREACT 136:37605; MARPAT 136:37605
 GI

L10 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2002 ACS (Continued)



AB The invention relates to methods of synthesizing 2-substituted asole compds. I and II (X = NH, NRA, S; ring H = 5 membered (un)substituted arom. ring structure contg. 0 - 2 addnl. heteroatoms selected from N, O, S provided that the addnl. heteroatoms are not at the attachment point of the R2 group; R2 = C2R3R4; Z = H, OH, alkoxy, amino, aminoalkoxy, etc.; R3 = H, alkyl, aralkyl, cycloalkyl, fluorinated alkyl, acyl, carboxy, carboxamide, etc.; R4 = alkyl, aryl, aralkyl, cycloalkyl, fluorinated alkyl, alkenyl, alkynyl, carboxy, etc.; RA = H, acyl, sulfonyl, carboxamide, etc.; ring A is a (un)satd. (arom.) 6-membered ring). The method involves prepn. key intermediate (optionally fused) III [S = solid support], cleaving the resin by nucleophilic substitution to yield I and optionally further substituting I via alkylation reactions in soln. phase. Data for over 100 compds. is provided. For instance, a polystyrene-carbonyl chloride resin (prepn. given) was combined with N-methylimidazole (5 mol equiv.) and benzaldehyde (10 mol equiv.) (1-Pr2NET, room temp., 24 h) to give a resin bound imidazole. This intermediate was cleaved (THF, TFA, water, 65.degree.C, 24 h) to give IV which was purified by chromatog.

can't make db. b/c is a no

L10 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:640817 CAPLUS
TITLE: Novel traceless solid-phase synthesis of
2-substituted
azole
AUTHOR(S): Deng, Yijun; Klasta, Dennis J.
CORPORATE SOURCE: Drug Discovery, The R.W. Johnson Pharmaceutical
Research Institute, Spring House, PA, 19477,
USA
SOURCE: Abstracts of Papers, 222nd ACS National
Meeting,
Chicago, IL, United States, August 26-30, 2001
(2001),
Washington, D.
ORGN-454. American Chemical Society:
C.
CODEN: 69BUZP
DOCUMENT TYPE: Conference; Meeting Abstract
LANGUAGE: English
AB Azoles, such as imidazole, are important heterocycle scaffolds
occurring in many drugs and biol. active compds. In the
accompanying
abstr., we describe a new reaction for the synthesis of
2-substituted
azoles via an azolium ylide. This reaction is ideal for
application to the traceless solid-phase synthesis of azole
libraries for high throughput screening. In two reaction steps,
azoles are formed with three centers of diversity that are arrayed
in a compact structure around a single carbon atom. We have found
that in
one step 2-substituted azoles (I) are assembled on resin by
using a resin bound acid chloride. Solvolysis conditions result in
cleavage of the azole off the resin, presumably in the form of a
carbonium ion, which is then trapped with a variety of
nucleophiles. This
two step sequence affords a library of 2-substituted azoles (II)
with at least three centers of diversity.

L10 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:640398 CAPLUS
TITLE: New synthesis of 2-substituted azoles via a
three-component one-pot reaction
AUTHOR(S): Deng, Yijun; Klaster, Dennis J.
CORPORATE SOURCE: Drug Discovery, The R.W. Johnson Pharmaceutical
Research Institute, Spring House, PA, 19477,
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SOURCE: Abstracts of Papers, 222nd ACS National
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Moreover, we found that the product (I) is readily transformed by
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solvolysis/displacement chem. into a wide range of functionalized
azole derivs. (II). Our recent results in developing new aspects
and the scope of this reaction will be described.

ND

=> fil reg
COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE	TOTAL
ENTRY	SESSION
43.94	188.43

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

CA SUBSCRIBER PRICE

SINCE FILE	TOTAL
ENTRY	SESSION
-6.82	-6.82

FILE 'REGISTRY' ENTERED AT 15:02:15 ON 25 OCT 2002
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STRUCTURE FILE UPDATES: 23 OCT 2002 HIGHEST RN 464874-85-9
DICTIONARY FILE UPDATES: 23 OCT 2002 HIGHEST RN 464874-85-9

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP
PROPERTIES for more information. See STNote 27, Searching Properties
in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=>
Uploading 09862808 electb.str

L12 STRUCTURE UPLOADED

=> d
L12 HAS NO ANSWERS
L12 STR

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L12          STRUCTURE UPLOADED
L13          5 S L12 FUL

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=> s 113 not 12
L14 0 L13 NOT L2

=> log y
COST IN U.S. DOLLARS

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

CA SUBSCRIBER PRICE

SINCE FILE	TOTAL
ENTRY	SESSION
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SINCE FILE	TOTAL
ENTRY	SESSION
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STN INTERNATIONAL LOGOFF AT 15:03:03 ON 25 OCT 2002